ACCESS DB # 287600

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Scientific and Technical Info[illegible]

SEARCH REQUES[illegible]

Requester's Full Name: Robinson Binta Exam[illegible]

Art Unit: 1625 Phone Number: 2-0692 Serial Number: 10583635

Location (Bldg/Room#): 4A70 (Mailbox #): _____ Results Format Preferred (circle): PAPER DISK

MG

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: Process for the manufacture of 2,3-dichloropyridine

Inventors (please provide full names): Rafael Shapiro

Earliest Priority Date: 1/23/04

Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known.

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

See claims 1-27

=> file registry
FILE 'REGISTRY' ENTERED AT 12:46:08 ON 06 MAR 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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provided by InfoChem.

STRUCTURE FILE UPDATES: 4 MAR 2009 HIGHEST RN 1115640-24-8
DICTIONARY FILE UPDATES: 4 MAR 2009 HIGHEST RN 1115640-24-8

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> file zcaplus
FILE 'ZCAPLUS' ENTERED AT 12:46:11 ON 06 MAR 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 6 Mar 2009 VOL 150 ISS 11
FILE LAST UPDATED: 5 Mar 2009 (20090305/ED)

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L64
L2 9 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON (1317-38-0/BI OR 2402-77-9/BI OR 462-08-8/BI OR 6298-19-7/BI OR 73074-20-1/BI OR 7447-39-4/BI OR 7632-00-0/BI OR 94770-75-9/BI OR 98-92-0/BI)

L3 1 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON 2402-77-9
L4 6 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L2 AND NC5/ES
L5 5 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L4 NOT L3
L9 572 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON (462-08-8/CRN OR 6298-19-7/CRN OR 73074-20-1/CRN OR 94770-75-9/CRN OR 98-92-0/CR

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                 1001003-91-3/CRN OR 1001003-97-9/CRN OR 16110-09-1/CRN OR
                 2402-77-9/CRN OR 2402-78-0/CRN OR 2457-47-8/CRN OR 25586-45-2/C
                 RN OR 26452-80-2/CRN OR 55934-00-4/CRN OR 70735-32-9/CRN OR
                 851516-88-6/CRN OR 98136-41-5/CRN)
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L29          151 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L28 AND NC5/ES
L42          721 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L11 OR L29
L43          721 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L42 AND NC5/ES
L62          866 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  SHAPIRO R?/AU
L64            4 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  (L27 OR L43) AND L62


=> d ibib abs hitstr L64 1-4

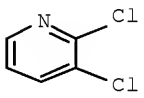
L64  ANSWER 1 OF 4  ZCAPLUS  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:         2005:696875  ZCAPLUS  Full-text
DOCUMENT NUMBER:          143:155307
TITLE:                    Process for the manufacture of 2,3-dichloropyridine
INVENTOR(S):              Shapiro, Rafael
PATENT ASSIGNEE(S):       E.I. Dupont de Nemours and Company, USA
SOURCE:                   PCT Int. Appl., 23 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.          DATE
     ---------------      ----   --------    --------------------     --------
     WO 2005070888         A2    20050804    WO 2005-US2462           20050121
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
             RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
             MR, NE, SN, TD, TG
     AU 2005206576         A1    20050804    AU 2005-206576           20050121
     CA 2553850            A1    20050804    CA 2005-2553850          20050121
     EP 1706381            A2    20061004    EP 2005-712075           20050121
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS, YU
     CN 1910152            A     20070207    CN 2005-80002691         20050121
     BR 2005006502         A     20070227    BR 2005-6502             20050121
     JP 2007523065         T     20070816    JP 2006-551437           20050121
     US 20070161797        A1    20070712    US 2006-583635           20060620
     IN 2006DN03640        A     20070824    IN 2006-DN3640           20060623
     MX 2006008208         A     20060831    MX 2006-8208             20060719
     KR 2006130618         A     20061219    KR 2006-714736           20060721
```

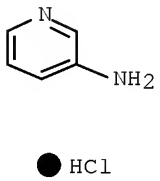
PRIORITY APPLN. INFO.: US 2004-539068P P 20040123
WO 2005-US2462 W 20050121
OTHER SOURCE(S): CASREACT 143:155307

AB A method for preparing 2,3-dichloropyridine is disclosed in which 3-amino-2-chloropyridine is contacted with an alkali metal nitrite in the presence of aqueous hydrochloric acid to form a diazonium salt; and the diazonium salt is subsequently decomposed in the presence of copper catalyst wherein at least about 50% of the copper is the copper(II) oxidation state.

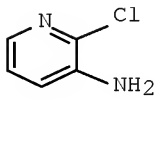
IT 2402-77-9P, 2,3-Dichloropyridine
RL: IMF (Industrial manufacture); PREP (Preparation)
(process for the manufacture of 2,3-dichloropyridine)
RN 2402-77-9 ZCAPLUS
CN Pyridine, 2,3-dichloro- (CA INDEX NAME)



IT 73074-20-1P, 3-Aminopyridine hydrochloride 94770-75-9P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(process for the manufacture of 2,3-dichloropyridine)
RN 73074-20-1 ZCAPLUS
CN 3-Pyridinamine, hydrochloride (1:1) (CA INDEX NAME)

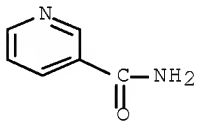


RN 94770-75-9 ZCAPLUS
CN 3-Pyridinamine, 2-chloro-, hydrochloride (1:1) (CA INDEX NAME)

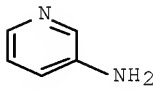


IT 98-92-0, Nicotinamide 462-08-8, 3-Aminopyridine
6298-19-7, 3-Amino-2-chloropyridine
RL: RCT (Reactant); RACT (Reactant or reagent)
(process for the manufacture of 2,3-dichloropyridine)
RN 98-92-0 ZCAPLUS

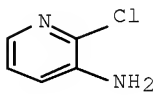
CN 3-Pyridinecarboxamide (CA INDEX NAME)



RN 462-08-8 ZCAPLUS
CN 3-Pyridinamine (CA INDEX NAME)



RN 6298-19-7 ZCAPLUS
CN 3-Pyridinamine, 2-chloro- (CA INDEX NAME)



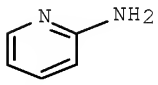
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 2 OF 4 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:301510 ZCAPLUS Full-text
DOCUMENT NUMBER: 133:104837
TITLE: Using Intelligent/Random Library Screening To Design Focused Libraries for the Optimization of Homogeneous Catalysts: Ullmann Ether Formation
AUTHOR(S): Fagan, Paul J.; Hauptman, Elisabeth; Shapiro, Rafael; Casalnuovo, Albert
CORPORATE SOURCE: Central Research and Development Department, The Dupont Company, Wilmington, DE, 19880-0328, USA
SOURCE: Journal of the American Chemical Society (2000), 122(21), 5043-5051
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:104837
AB A 96-member pyridine library consisting of both rationally chosen and random members was used to screen Ullmann ether forming reactions. The reaction of 2-bromo-4,6-dimethylaniline and other substrates with a variety of alkoxides was studied under different conditions with the aid of an automated liquid handler. From the results of the 96-member library screening, a structure activity profile was determined which led to the design of smaller focused

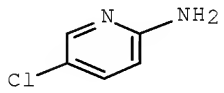
ligand libraries. The focused libraries produced a higher frequency of hits compared to the original 96-member library. Some of the more effective ligands discovered in this work are generally useful for alkoxylation of a variety of substrates, and also functioned in intramol. ether forming reactions. This work demonstrates for homogeneous catalysis the analogy to the pharmacol. model of drug discovery. By using a large library to screen for a lead compound followed by screening the diversity space closest to the lead, a larger fraction of increased performance ligands was discovered.

IT 504-29-0, 2-Aminopyridine 1072-98-6, 2-Amino-5-chloropyridine 1452-77-3, Picolinamide 1453-82-3, Isonicotinamide 34813-97-3
RL: CAT (Catalyst use); USES (Uses)
(optimization of pyridine ligand components for catalytic Ullmann alkoxylation)

RN 504-29-0 ZCAPLUS
CN 2-Pyridinamine (CA INDEX NAME)



RN 1072-98-6 ZCAPLUS
CN 2-Pyridinamine, 5-chloro- (CA INDEX NAME)



RN 1452-77-3 ZCAPLUS
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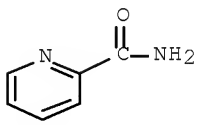
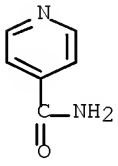
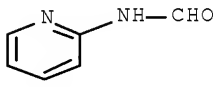


RN 1453-82-3 ZCAPLUS
CN 4-Pyridinecarboxamide (CA INDEX NAME)



RN 34813-97-3 ZCAPLUS
CN Formamide, N-2-pyridinyl- (CA INDEX NAME)



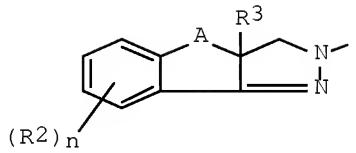
REFERENCE COUNT: 112 THERE ARE 112 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 3 OF 4 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:35002 ZCAPLUS Full-text
DOCUMENT NUMBER: 124:202246
ORIGINAL REFERENCE NO.: 124:37393a,37396a
TITLE: Arthropodicidal pyrazolines, pyrazolidines and hydrazines
INVENTOR(S): Harrison, Charles R.; Lett, Renee M.; Mccann, Stephen F.; Shapiro, Rafael; Stevenson, Thomas M.
PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
SOURCE: U.S., 64 pp. Cont.-in-part of U.S. Ser. No. 569,044, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5474998	A	19951212	US 1993-971974	19930216
WO 9203421	A2	19920305	WO 1991-US5334	19910801
WO 9203421	A3	19921029		
W: JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				

PRIORITY APPLN. INFO.:
US 1990-569044 B2 19900817
US 1990-573954 B2 19900827
US 1990-595151 B2 19901009
WO 1991-US5334 W 19910801

OTHER SOURCE(S): MARPAT 124:202246
GI



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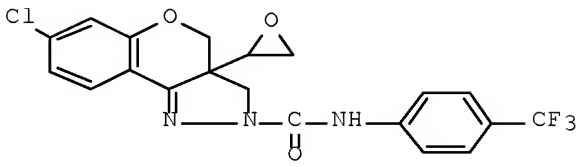


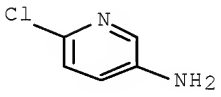
II

AB Arthropodicidal pyrazoline, pyrazolidine and hydrazine compds. are claimed, including all their geometric and stereoisomers, agriculturally suitable salts thereof and compns. containing them, and a method for controlling arthropods employing said compds. which are QC(:X)NYG and QCX1:NG wherein Q = e.g., I with A = e.g., CH2, CH2CH2, O, OCH2; R2 = e.g., H, C1-6 alkyl, C1-6 haloalkyl; R3 = e.g., H, CN, epoxyalkyl; n = 1-3; G = e.g., (un)substituted pyridyl, pyrimidinyl, Ph; X = e.g., O, S; X1 = e.g., Cl, Br; Y = e.g., H, C1-6 alkyl, benzyl. Thus, e.g., epoxidn. of 7-chloro-3a-ethenyl-2,3,3a,4-tetrahydro-N-[4-(trifluoromethyl)phenyl][1]benzopyrano[4,3-c]pyrazole-2-carboxamide afforded two oxiranyl diastereomers II which exhibited mortality levels of 80% or higher against, e.g., tobacco budworm, aster leafhopper, and boll weevil at 0.55 kg/ha.

IT 5350-93-6, 5-Amino-2-chloropyridine
RL: RCT (Reactant); RACT (Reactant or reagent)
(arthropodicidal pyrazolines, pyrazolidines and hydrazines)

RN 5350-93-6 ZCAPLUS

CN 3-Pyridinamine, 6-chloro- (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 4 OF 4 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1992:426559 ZCAPLUS Full-text

DOCUMENT NUMBER: 117:26559

ORIGINAL REFERENCE NO.: 117:4803a,4806a

TITLE: Preparation of arthropodicidal benzopyranopyrazolecarboxamides, -carboxylates, and related compounds

INVENTOR(S): Harrison, Charles Richard; Lett, Renee Marie; McCann, Stephen Frederick; Shapiro, Rafael; Stevenson, Thomas Martin

PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co., USA

SOURCE: PCT Int. Appl., 291 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9203421	A2	19920305	WO 1991-US5334	19910801
WO 9203421	A3	19921029		
W: JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
EP 543930	A1	19930602	EP 1991-916421	19910801
R: DE, ES, FR, GB, IT				
JP 06500333	T	19940113	JP 1991-515611	19910801
US 5474998	A	19951212	US 1993-971974	19930216
PRIORITY APPLN. INFO.:			US 1990-569044 A2	19900817
			US 1990-573954 A2	19900827
			US 1990-595151 A2	19901009
			WO 1991-US5334 W	19910801

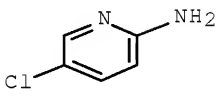
OTHER SOURCE(S): MARPAT 117:26559
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

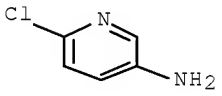
AB The title compds. QC(:X)N(Y)G and QC(X1)(:NG) [Q = Q1-Q5; A = CH2, CH2CH2, O, S, NR5, etc.; G = (un)substituted pyridinyl, -pyrimidinyl, -phenyl(amino), etc.; X = O, S, NX2; X1 = Cl, Br, OR6, etc.; X2 = HO, cyano, SO2Ph, R6, etc.; Y, Y1 = H, C1-6 alkyl(thio), C2-6 alkoxycarbonyl, PhCH2, CHO, etc.; Z (un)substituted = (CH2)q, CH2OCH2, etc.; V = O, S, NR5, R2 = H, C1-6 (halo)alkyl, C2-6 (halo)alkenyl, cyano, NO2, etc.; R3 = Ra, Rb, J; Ra = H, C1-6 (halo)alkyl; Rb = cyano, azido, etc.; J = (un)saturated 5- or 6-membered (un)substituted heteroring; R4 = H, C1-6 (halo)alkyl, (un)substituted Ph, etc.; R5 = H, C1-6 (halo)alkyl, S(O)R15, etc.; R6 = C1-3 alkyl, (un)substituted benzyl, etc.; R15 = H, C1-6 (halo)alkyl, (un)substituted Ph, etc.; R18 = H, C1-4 (halo)alkyl, C4-7 alkylcycloalkyl, etc.; R19 = H, C1-3 alkyl, CO2R15, etc.; R32 = H, Me, CO2Me; n = 1-3, q = 2-4; with a proviso] were prepared as pesticides. Condensation of 2-acetyl-5-chlorothiophene with MeMgBr in Et2O followed by dehydration of the intermediate carbinol gave 2-chloro-5-(1-methylethenyl)thiophene. This was chlorinated by NBS/(PhSe)2 in CH2Cl2/pyridine, the mixture of the resulting vinylic and allylic chlorides in DMF was etherified with 4,2-CF3(HO)C6H3CHO, and the product chromatographed to give 2-[[2-(5-chloro-2-thienyl)-2-propenyl]oxy]- 4-(trifluoromethyl)benzaldehyde. The aldehyde was condensed with (EtO)2P(O)NHNH2 in EtOH, the hydrazide cyclized by NBS/Et3N in CH2Cl2, the resulting (benzopyranopyrazolyl)phosphonate was dephosphorylated by Me3SiCl in EtOH, and condensed with 4-CF3C6H4NCO in CH2Cl2 to give title compound (I). I at .apprx.0.55 kg/ha killed ≥80% 3d-instar larvae of Spodoptera frugiperda, Heliothis virescens, and Diabrotica undecimpunctata.

IT 1072-98-6, 2-Amino-5-chloropyridine 5350-93-6, 5-Amino-2-chloropyridine
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of, in preparation of pesticides)

RN 1072-98-6 ZCAPLUS
CN 2-Pyridinamine, 5-chloro- (CA INDEX NAME)



RN 5350-93-6 ZCAPLUS
CN 3-Pyridinamine, 6-chloro- (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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STRUCTURE FILE UPDATES:    4 MAR 2009  HIGHEST RN 1115640-24-8
DICTIONARY FILE UPDATES:   4 MAR 2009  HIGHEST RN 1115640-24-8

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  Please note that search-term pricing does apply when
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=> file zcaplus
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FILE COVERS 1907 - 6 Mar 2009  VOL 150 ISS 11
FILE LAST UPDATED: 5 Mar 2009  (20090305/ED)

ZCAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L13
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L2            9 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (1317-38-0/BI OR
                2402-77-9/BI OR 462-08-8/BI OR 6298-19-7/BI OR 73074-20-1/BI
                OR 7447-39-4/BI OR 7632-00-0/BI OR 94770-75-9/BI OR 98-92-0/BI)

L3            1 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  2402-77-9
L4            6 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L2 AND NC5/ES
L5            5 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L4 NOT  L3
L8            1 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  2402-77-9/CRN
L9          572 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (462-08-8/CRN OR
                6298-19-7/CRN OR 73074-20-1/CRN OR 94770-75-9/CRN OR 98-92-0/CR
                N)
L10           2 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L8 OR L3
L11         575 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L9 OR L5
L12          23 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L10 (L) PREP/RL
L13           5 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L11 AND L12


=> d stat que L21
L2            9 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (1317-38-0/BI OR
                2402-77-9/BI OR 462-08-8/BI OR 6298-19-7/BI OR 73074-20-1/BI
                OR 7447-39-4/BI OR 7632-00-0/BI OR 94770-75-9/BI OR 98-92-0/BI)

L3            1 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  2402-77-9
L4            6 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L2 AND NC5/ES
L5            5 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L4 NOT  L3
L8            1 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  2402-77-9/CRN
L9          572 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (462-08-8/CRN OR
                6298-19-7/CRN OR 73074-20-1/CRN OR 94770-75-9/CRN OR 98-92-0/CR
                N)
L10           2 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L8 OR L3
L11         575 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L9 OR L5
L12          23 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L10 (L) PREP/RL
L13           5 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L11 AND L12
L14      544228 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  CU/ELS
L15             TRANSFER  PLU=ON  L13 1- RN :      99 TERMS
L16          99 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L15
L17           5 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L14 AND L16
L18       14680 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  ?NITRIT?/CNS
L19           1 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L16 AND L18
L21           2 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L13 AND (L17 OR L19)


=> d stat que L22
L2            9 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (1317-38-0/BI OR
                2402-77-9/BI OR 462-08-8/BI OR 6298-19-7/BI OR 73074-20-1/BI
                OR 7447-39-4/BI OR 7632-00-0/BI OR 94770-75-9/BI OR 98-92-0/BI)

L3            1 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  2402-77-9
L4            6 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L2 AND NC5/ES
L5            5 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L4 NOT  L3
L8            1 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  2402-77-9/CRN
L9          572 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (462-08-8/CRN OR
                6298-19-7/CRN OR 73074-20-1/CRN OR 94770-75-9/CRN OR 98-92-0/CR
                N)
L10           2 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L8 OR L3
L11         575 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L9 OR L5
L12          23 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L10 (L) PREP/RL
L13           5 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L11 AND L12
L22           3 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L13 AND (CU/BI OR
                COPPER?/BI OR CUPR?/BI)
```

```
=> d stat que L36
L2             9 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (1317-38-0/BI OR
                 2402-77-9/BI OR 462-08-8/BI OR 6298-19-7/BI OR 73074-20-1/BI
                 OR 7447-39-4/BI OR 7632-00-0/BI OR 94770-75-9/BI OR 98-92-0/BI)

L3             1 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  2402-77-9
L4             6 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L2 AND NC5/ES
L5             5 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L4 NOT  L3
L14       544228 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  CU/ELS
L23           16 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  C5H3CL2N/MF
L26          109 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (1001003-85-5/CRN OR
                 1001003-86-6/CRN OR 1001003-87-7/CRN OR 1001003-88-8/CRN OR
                 1001003-91-3/CRN OR 1001003-97-9/CRN OR 16110-09-1/CRN OR
                 2402-77-9/CRN OR 2402-78-0/CRN OR 2457-47-8/CRN OR 25586-45-2/C
                 RN OR 26452-80-2/CRN OR 55934-00-4/CRN OR 70735-32-9/CRN OR
                 851516-88-6/CRN OR 98136-41-5/CRN)
L27          125 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L23 OR L26
L28          571 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (C5H5CLN2.CLH/MF OR
                 C5H5CLN2/MF OR C5H6N2.CLH/MF OR C5H6N2/MF OR C6H6N2O/MF)
L29          151 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L28 AND NC5/ES
L30          151 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L5 OR L29
L31          209 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L27 (L) PREP/RL
L32           23 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L30 AND L31
L33              TRANSFER  PLU=ON  L32 1- RN :    7677 TERMS
L34         7677 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L33
L35            6 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L34 AND L14
L36            3 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L32 AND L35


=> d stat que L39
L2             9 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (1317-38-0/BI OR
                 2402-77-9/BI OR 462-08-8/BI OR 6298-19-7/BI OR 73074-20-1/BI
                 OR 7447-39-4/BI OR 7632-00-0/BI OR 94770-75-9/BI OR 98-92-0/BI)

L3             1 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  2402-77-9
L4             6 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L2 AND NC5/ES
L5             5 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L4 NOT  L3
L23           16 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  C5H3CL2N/MF
L26          109 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (1001003-85-5/CRN OR
                 1001003-86-6/CRN OR 1001003-87-7/CRN OR 1001003-88-8/CRN OR
                 1001003-91-3/CRN OR 1001003-97-9/CRN OR 16110-09-1/CRN OR
                 2402-77-9/CRN OR 2402-78-0/CRN OR 2457-47-8/CRN OR 25586-45-2/C
                 RN OR 26452-80-2/CRN OR 55934-00-4/CRN OR 70735-32-9/CRN OR
                 851516-88-6/CRN OR 98136-41-5/CRN)
L27          125 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L23 OR L26
L28          571 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (C5H5CLN2.CLH/MF OR
                 C5H5CLN2/MF OR C5H6N2.CLH/MF OR C5H6N2/MF OR C6H6N2O/MF)
L29          151 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L28 AND NC5/ES
L30          151 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L5 OR L29
L31          209 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L27 (L) PREP/RL
L32           23 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L30 AND L31
L37            7 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L32 AND (CU/BI OR
                 COPPER?/BI OR CUPR?/BI)
L38         9735 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L30 (L) RACT/RL
L39            3 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L38 AND L37


=> d stat que L51
```

```
L2            9 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (1317-38-0/BI OR
                2402-77-9/BI OR 462-08-8/BI OR 6298-19-7/BI OR 73074-20-1/BI
                OR 7447-39-4/BI OR 7632-00-0/BI OR 94770-75-9/BI OR 98-92-0/BI)

L3            1 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  2402-77-9
L4            6 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L2 AND NC5/ES
L5            5 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L4 NOT  L3
L9          572 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (462-08-8/CRN OR
                6298-19-7/CRN OR 73074-20-1/CRN OR 94770-75-9/CRN OR 98-92-0/CR
                N)
L11         575 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L9 OR L5
L23          16 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  C5H3CL2N/MF
L26         109 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (1001003-85-5/CRN OR
                1001003-86-6/CRN OR 1001003-87-7/CRN OR 1001003-88-8/CRN OR
                1001003-91-3/CRN OR 1001003-97-9/CRN OR 16110-09-1/CRN OR
                2402-77-9/CRN OR 2402-78-0/CRN OR 2457-47-8/CRN OR 25586-45-2/C
                RN OR 26452-80-2/CRN OR 55934-00-4/CRN OR 70735-32-9/CRN OR
                851516-88-6/CRN OR 98136-41-5/CRN)
L27         125 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L23 OR L26
L28         571 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (C5H5CLN2.CLH/MF OR
                C5H5CLN2/MF OR C5H6N2.CLH/MF OR C5H6N2/MF OR C6H6N2O/MF)
L29         151 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L28 AND NC5/ES
L31         209 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L27 (L) PREP/RL
L42         721 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L11 OR L29
L43         721 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L42 AND NC5/ES
L50        9763 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L43 (L) RACT/RL
L51           5 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L50 AND L31


=> s L13 or L21 or L22 or L36 or L51 or L39
L65           8 L13 OR L21 OR L22 OR L36 OR L51 OR L39

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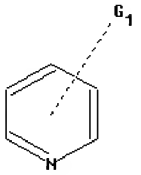

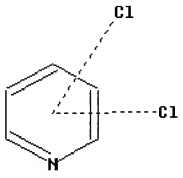

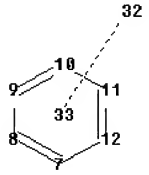

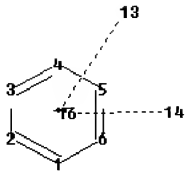

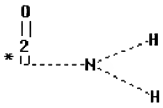

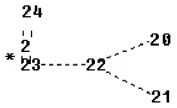

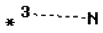

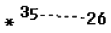

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ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
17-18 17-19 20-22 21-22 22-23 23-24 25-26
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
17-18 17-19 20-22 21-22 22-23 23-24 25-26
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

G1:[*1],[*2],[*3]

Connectivity :
25:2 E exact RC ring/chain 26:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 32:CLASS 33:CLASS
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containing 1
fragments assigned reactant/reagent role:
containing 7
node mappings:
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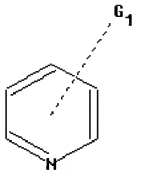
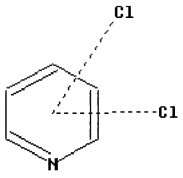
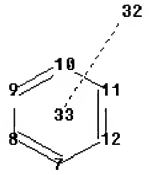
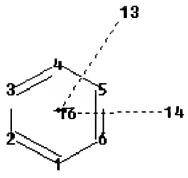
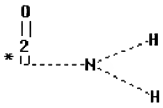
Uploading L58.str

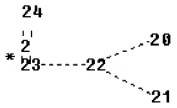


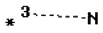


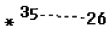












chain nodes :
13 14 17 18 19 20 21 22 23 24 25 26 32
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
17-18 17-19 20-22 21-22 22-23 23-24 25-26
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
17-18 17-19 20-22 21-22 22-23 23-24 25-26
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

G1:[*1],[*2],[*3]

Connectivity :
25:2 E exact RC ring/chain 26:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 32:CLASS 33:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 7
reaction site bonds:
13-15:CC

```
node mappings:
1:7




=> => d stat que L67
L52             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L54       30743 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  CU/ELS AND CASREACT/L
                C
L55       51052 SEA FILE=CASREACT SPE=ON  ABB=ON  PLU=ON  L54
L57          12 SEA FILE=CASREACT SUB=L55 SSS FUL L52 (    77 REACTIONS)
L58             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L60           5 SEA FILE=CASREACT SUB=L57 SSS FUL L58 (    12 REACTIONS)
L67           5 SEA FILE=CASREACT SPE=ON  ABB=ON  PLU=ON  L55 (L) L60


=> dup rem L67 L65
FILE 'CASREACT' ENTERED AT 12:49:21 ON 06 MAR 2009
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2009 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'ZCAPLUS' ENTERED AT 12:49:21 ON 06 MAR 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2009 AMERICAN CHEMICAL SOCIETY (ACS)
PROCESSING COMPLETED FOR L67
PROCESSING COMPLETED FOR L65
L68           11 DUP REM L67 L65 (2 DUPLICATES REMOVED)
                 ANSWERS '1-5' FROM FILE CASREACT
                 ANSWERS '6-11' FROM FILE ZCAPLUS

=> d ibib abs hit L68 1-5; d ibib abs hitind hitstr L68 6-11

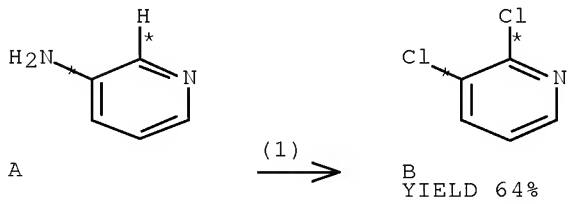

L68  ANSWER 1 OF 11  CASREACT  COPYRIGHT 2009 ACS on STN DUPLICATE 1
ACCESSION NUMBER:        145:188734  CASREACT  Full-text
TITLE:                   Preparation method for 2,3-dichloropyridine from
                         3-aminopyridine
INVENTOR(S):             Zhao, Taolin; Liu, Aiguo
PATENT ASSIGNEE(S):      Nanjing Guangtong Pharmaceutical and Chemical Co.,
                         Ltd., Peop. Rep. China
SOURCE:                  Faming Zhuanli Shenqing Gongkai Shuomingshu, 7 pp.
                         CODEN: CNXXEV
DOCUMENT TYPE:           Patent
LANGUAGE:                Chinese
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.       KIND  DATE           APPLICATION NO.  DATE
     ---------------  ----  --------       ---------------  --------
```

CN 1807414 A 20060726 CN 2006-10038159 20060206
CN 100357272 C 20071226
PRIORITY APPLN. INFO.: CN 2006-10038159 20060206

AB The title preparation method includes 2-chlorination of 3-aminopyridine with hydrogen peroxide (content <20%) at a molar ratio of 1:1 in concentrated hydrochloric acid (content ≤31%) at 6-8 ℃ for 1-2 h; diazotizing with 30% sodium nitrite solution (at equal mole to the 3-aminopyridine) at <0 ℃ for 0.5-1 h; 3-chlorination with mixture of cuprous chloride (0.15 M times of 3-aminopyridine) and concentrated hydrochloric acid (2 M times of 3-aminopyridine) at <0 ℃ for >30 min; extracting with dichloromethane at room temperature; and vacuum distilling solvent out to obtain 2,3-dichloropyridine.

RX(1) OF 1 A ===> B



RX(1) RCT A 462-08-8

STAGE(1)
RGT C 7647-01-0 HCl, D 7722-84-1 H2O2
SOL 7732-18-5 Water
CON SUBSTAGE(1) room temperature -> 30 deg C
SUBSTAGE(2) 30 deg C -> 4 deg C
SUBSTAGE(3) 52 minutes, 6 - 8 deg C
SUBSTAGE(4) 1 hour, 6 - 8 deg C
SUBSTAGE(5) 8 deg C -> -8 deg C

STAGE(2)
RGT E 7632-00-0 NaNO2
SOL 7732-18-5 Water
CON SUBSTAGE(1) 25 minutes, -8 - -5 deg C
SUBSTAGE(2) 30 minutes, -8 - -5 deg C
SUBSTAGE(3) -5 deg C -> -10 deg C

STAGE(3)
RGT C 7647-01-0 HCl
CAT 7758-89-6 CuCl
SOL 7732-18-5 Water
CON SUBSTAGE(1) 63 minutes, -10 - -5 deg C
SUBSTAGE(2) 1 hour, -5 - 0 deg C
SUBSTAGE(3) 0 deg C -> room temperature

PRO B 2402-77-9
NTE regioselective, optimization study, optimized on the reaction temperature and time

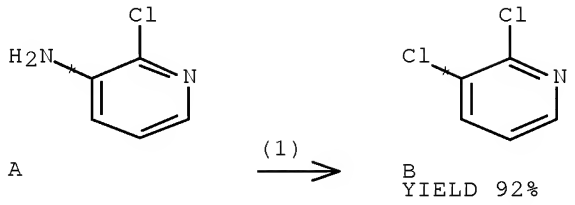
L68 ANSWER 2 OF 11 CASREACT COPYRIGHT 2009 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 143:155307 CASREACT Full-text
TITLE: Process for the manufacture of 2,3-dichloropyridine
INVENTOR(S): Shapiro, Rafael
PATENT ASSIGNEE(S): E.I. Dupont de Nemours and Company, USA
SOURCE: PCT Int. Appl., 23 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005070888	A2	20050804	WO 2005-US2462	20050121
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005206576	A1	20050804	AU 2005-206576	20050121
CA 2553850	A1	20050804	CA 2005-2553850	20050121
EP 1706381	A2	20061004	EP 2005-712075	20050121
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS, YU				
CN 1910152	A	20070207	CN 2005-80002691	20050121
BR 2005006502	A	20070227	BR 2005-6502	20050121
JP 2007523065	T	20070816	JP 2006-551437	20050121
US 20070161797	A1	20070712	US 2006-583635	20060620
IN 2006DN03640	A	20070824	IN 2006-DN3640	20060623
MX 2006008208	A	20060831	MX 2006-8208	20060719
KR 2006130618	A	20061219	KR 2006-714736	20060721
PRIORITY APPLN. INFO.:			US 2004-539068P	20040123
			WO 2005-US2462	20050121

AB A method for preparing 2,3-dichloropyridine is disclosed in which 3-amino-2-chloropyridine is contacted with an alkali metal nitrite in the presence of aqueous hydrochloric acid to form a diazonium salt; and the diazonium salt is subsequently decomposed in the presence of copper catalyst wherein at least about 50% of the copper is the copper(II) oxidation state.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 11 ...A ===> B



RX(1) RCT A 6298-19-7

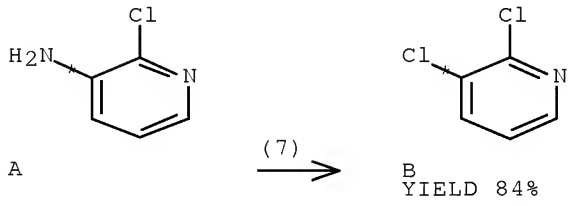
STAGE(1)
RGT C 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature -> -8 deg C

STAGE(2)
RGT D 7632-00-0 NaNO2
SOL 7732-18-5 Water
CON 30 minutes, -7 - -3 deg C

STAGE(3)
RGT C 7647-01-0 HCl
CAT 1317-38-0 CuO
SOL 109-69-3 BuCl, 7732-18-5 Water
CON 55 - 62 deg C

PRO B 2402-77-9

RX(7) OF 11 A ===> B



RX(7) RCT A 6298-19-7

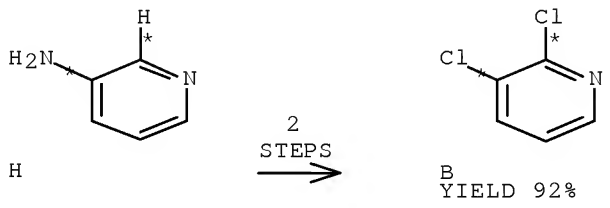
STAGE(1)
RGT D 7632-00-0 NaNO2
SOL 7732-18-5 Water
CON 30 minutes, -5 - 0 deg C

STAGE(2)
RGT C 7647-01-0 HCl
CAT 7447-39-4 CuCl2
SOL 109-69-3 BuCl, 7732-18-5 Water
CON SUBSTAGE(1) 1 hour, 60 deg C

SUBSTAGE(2) 30 minutes, 60 deg C

PRO B 2402-77-9

RX(8) OF 11 COMPOSED OF RX(2), RX(1)
RX(8) [illegible] ===> [illegible]



RX(2) RCT H 462-08-8

STAGE(1)
RGT C 7647-01-0 HCl
SOL 7732-18-5 Water
CON 30 - 35 deg C

STAGE(2)
RGT I 7722-84-1 H2O2
SOL 7732-18-5 Water
CON SUBSTAGE(1) 20 minutes, 10 - 12 deg C
SUBSTAGE(2) 2 hours, 10 deg C
SUBSTAGE(3) 2 hours, 10 deg C -> 19 deg C
SUBSTAGE(4) 4 hours, 19 deg C

STAGE(3)
RGT J 7757-83-7 Na2SO3
SOL 7732-18-5 Water
CON 10 deg C

STAGE(4)
RGT K 1310-73-2 NaOH
SOL 7732-18-5 Water, 108-88-3 PhMe
CON 25 - 35 deg C

PRO A 6298-19-7

RX(1) RCT A 6298-19-7

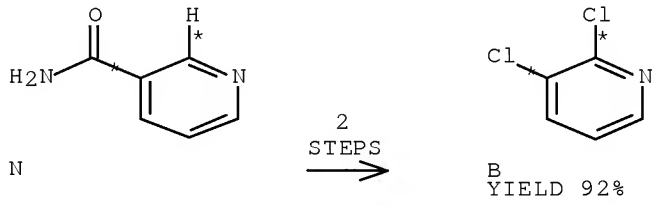
STAGE(1)
RGT C 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature -> -8 deg C

STAGE(2)
RGT D 7632-00-0 NaNO2
SOL 7732-18-5 Water
CON 30 minutes, -7 - -3 deg C

STAGE(3)
RGT C 7647-01-0 HCl
CAT 1317-38-0 CuO
SOL 109-69-3 BuCl, 7732-18-5 Water
CON 55 - 62 deg C

PRO B 2402-77-9

RX(9) OF 11 COMPOSED OF RX(4), RX(1)
RX(9) N ===> B



RX(4) RCT N 98-92-0

STAGE(1)
RGT O 7681-52-9 NaOCl
SOL 7732-18-5 Water
CON 30 minutes, 0 - 5 deg C

STAGE(2)
RGT K 1310-73-2 NaOH
SOL 7732-18-5 Water
CON 30 minutes, 0 - 5 deg C

STAGE(3)
SOL 7732-18-5 Water
CON SUBSTAGE(1) 40 minutes, 75 - 81 deg C
SUBSTAGE(2) 15 minutes, 80 deg C

STAGE(4)
RGT C 7647-01-0 HCl
SOL 7732-18-5 Water
CON 40 - 50 deg C

STAGE(5)
RGT I 7722-84-1 H2O2
SOL 7732-18-5 Water
CON SUBSTAGE(1) 1.5 hours, 10 deg C
SUBSTAGE(2) 2 hours, room temperature
SUBSTAGE(3) 30 minutes, room temperature

STAGE(6)
RGT K 1310-73-2 NaOH, J 7757-83-7 Na2SO3
SOL 7732-18-5 Water, 108-88-3 PhMe
CON 15 - 25 deg C

PRO A 6298-19-7

RX(1) RCT A 6298-19-7

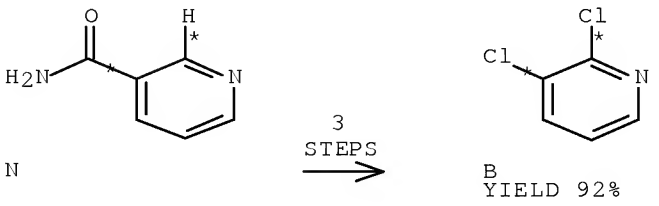
STAGE(1)
RGT C 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature -> -8 deg C

STAGE(2)
RGT D 7632-00-0 NaNO2
SOL 7732-18-5 Water
CON 30 minutes, -7 - -3 deg C

STAGE(3)
RGT C 7647-01-0 HCl
CAT 1317-38-0 CuO
SOL 109-69-3 BuCl, 7732-18-5 Water
CON 55 - 62 deg C

PRO B 2402-77-9

RX(11) OF 11 COMPOSED OF RX(5), RX(2), RX(1)
RX(11) N ===> B



RX(5) RCT N 98-92-0

STAGE(1)
RGT O 7681-52-9 NaOCl
SOL 7732-18-5 Water
CON SUBSTAGE(1) 30 minutes, 0 deg C
SUBSTAGE(2) 15 minutes, 0 deg C

STAGE(2)
RGT K 1310-73-2 NaOH
SOL 7732-18-5 Water
CON 30 minutes, 0 - 5 deg C

STAGE(3)
SOL 7732-18-5 Water
CON SUBSTAGE(1) 30 minutes, 90 deg C
SUBSTAGE(2) 1 hour, 90 deg C

STAGE(4)
RGT C 7647-01-0 HCl
SOL 7732-18-5 Water

```
              CON  SUBSTAGE(1) 45 minutes, 40 deg C
                   SUBSTAGE(2) overnight, room temperature

           PRO  H 462-08-8

RX(2)      RCT  H 462-08-8

             STAGE(1)
                RGT  C 7647-01-0 HCl
                SOL  7732-18-5 Water
                CON  30 - 35 deg C

             STAGE(2)
                RGT  I 7722-84-1 H2O2
                SOL  7732-18-5 Water
                CON  SUBSTAGE(1) 20 minutes, 10 - 12 deg C
                     SUBSTAGE(2) 2 hours, 10 deg C
                     SUBSTAGE(3) 2 hours, 10 deg C -> 19 deg C
                     SUBSTAGE(4) 4 hours, 19 deg C

             STAGE(3)
                RGT  J 7757-83-7 Na2SO3
                SOL  7732-18-5 Water
                CON  10 deg C

             STAGE(4)
                RGT  K 1310-73-2 NaOH
                SOL  7732-18-5 Water, 108-88-3 PhMe
                CON  25 - 35 deg C

           PRO  A 6298-19-7

RX(1)      RCT  A 6298-19-7

             STAGE(1)
                RGT  C 7647-01-0 HCl
                SOL  7732-18-5 Water
                CON  room temperature -> -8 deg C

             STAGE(2)
                RGT  D 7632-00-0 NaNO2
                SOL  7732-18-5 Water
                CON  30 minutes, -7 - -3 deg C

             STAGE(3)
                RGT  C 7647-01-0 HCl
                CAT  1317-38-0 CuO
                SOL  109-69-3 BuCl, 7732-18-5 Water
                CON  55 - 62 deg C

           PRO  B 2402-77-9

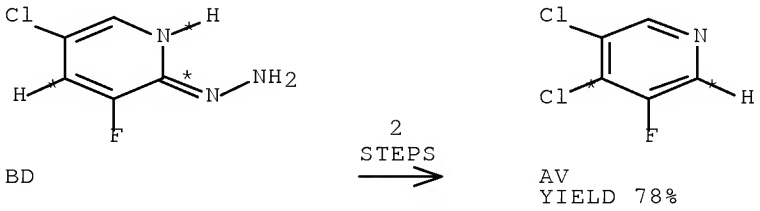

L68  ANSWER 3 OF 11  CASREACT  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:        142:447087  CASREACT  Full-text
TITLE:                   Removal of fluorine from and introduction of fluorine
                         into polyhalopyridines: an exercise in nucleophilic
                         hetarenic substitution
AUTHOR(S):               Bobbio, Carla; Rausis, Thierry; Schlosser, Manfred
CORPORATE SOURCE:        Institute of Chemical Sciences and Engineering, Ecole
```

Polytechnique Federale, Lausanne, 1015, Switz.
SOURCE: Chemistry--A European Journal (2005), 11(6), 1903-1910
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Starting from six industrially available fluorinated pyridines, an expedient access to all three tetrafluoropyridines, all six trifluoropyridines, and the five non-com. difluoropyridines was developed. The methods employed for the selective removal of fluorine from polyfluoropyridines were the reduction by metals or complex hydrides and the site-selective replacement by hydrazine followed by dehydrogenation-dediazotation or dehydrochlorination-dediazotation. To introduce an extra fluorine atom, a suitable precursor was metalated and chlorinated before being subjected to a chlorine/fluorine displacement process.

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(62) OF 136 COMPOSED OF RX(24), RX(23)
RX(62) BD ===> AV



BD

AV
YIELD 78%

RX(24) RCT BD 248255-70-1
RGT T 7758-98-7 CuSO4
PRO BC 514797-99-0
SOL 7732-18-5 Water
CON 2 hours, reflux

RX(23) RCT BC 514797-99-0

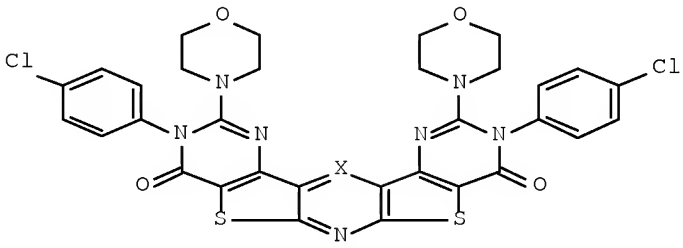
STAGE(1)
RGT AP 109-72-8 BuLi
SOL 109-99-9 THF, 110-54-3 Hexane
CON 2 hours, -75 deg C

STAGE(2)
RGT AW 76-13-1 Freon 113
CON 1 hour, -75 deg C

PRO AV 851179-02-7

L68 ANSWER 4 OF 11 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 140:163819 CASREACT Full-text
TITLE: Synthesis of pyrido and pyrazinodithienodipyrimidine-4,8(3H,9H)-dione derivatives by the aza-Wittig methodology

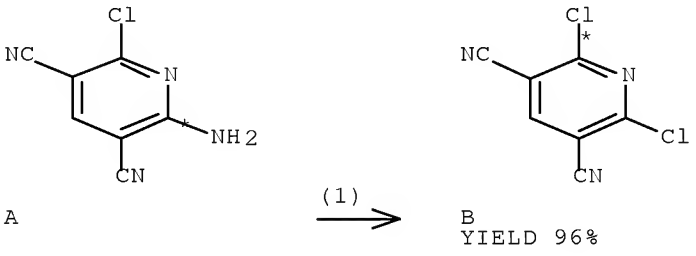
AUTHOR(S): Vilarelle, David Vazquez; Veira, Carlos Peinador; Quintela Lopez, Jose M.
CORPORATE SOURCE: Facultad de Ciencias, Departamento de Quimica Fundamental, Universidad de La Coruna, La Coruna, E-15071, Spain
SOURCE: Tetrahedron (2004), 60(2), 275-283
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB A one-pot synthesis of the hitherto unreported pyrido[5'',6'':4,5;3''2'':4',5']dithieno[3,2-d:3',2'-d']dipyrimidine-4,8(3H,9H)-diones, e.g. I (X = CH), and pyrazino[5'',6'':4,5;3''2'':4',5']dithieno[3,2-d:3',2'-d']dipyrimidine-4,8(3H,9H)-diones, e.g. I (X = N) pentaheterocyclic systems, based on the tandem aza-Wittig heterocumulene-mediated annulation strategy, is described.
REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 157 A ===> B...



A B
(1)
YIELD 96%

RX(1) RCT A 51768-01-5

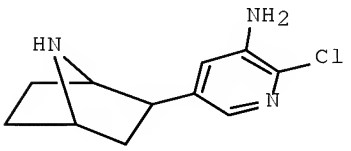
STAGE(1)
RGT C 7447-39-4 CuCl2, D 110-46-3 Isoamyl nitrite
SOL 75-05-8 MeCN

CON 5 hours, 65 deg C

STAGE(2)
RGT E 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature, acidify

PRO B 151229-84-4

L68 ANSWER 5 OF 11 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 137:353202 CASREACT Full-text
TITLE: Synthesis, Nicotinic Acetylcholine Receptor Binding, and Antinociceptive Properties of 2-exo-2-(2',3'-Disubstituted 5'-pyridinyl)-7-azabicyclo[2.2.1]heptanes: Epibatidine Analogues
AUTHOR(S): Carroll, F. Ivy; Lee, Jeffrey R.; Navarro, Hernan A.; Ma, Wei; Brieaddy, Lawrence E.; Abraham, Philip; Damaj, M. I.; Martin, Billy R.
CORPORATE SOURCE: Chemistry and Life Sciences, Research Triangle Institute, Research Triangle Park, NC, 27709, USA
SOURCE: Journal of Medicinal Chemistry (2002), 45(21), 4755-4761
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



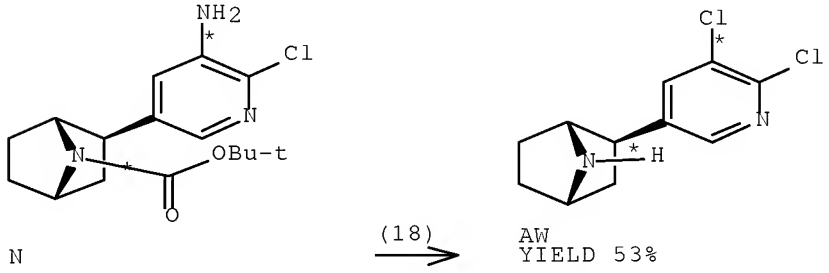
I

AB A number of 2',3'-disubstituted epibatidine analogs were synthesized and evaluated in vitro for potency at nicotinic acetylcholine receptors (nAChRs) and in vivo for antinociception activity in the tail-flick and hot-plate models of acute pain and for their ability to affect core body temperature Compds. that possessed electron-withdrawing groups (F, Cl, Br, and I) in both the 2'- and the 3'-positions showed affinities at the nAChR similar to epibatidine. However, in vivo efficacy did not correlate with affinity. 2-Exo-(3'-Amino-2'-chloro-5'-pyridinyl)-7- azabicyclo[2.2.1]heptane (I), an epibatidine analog possessing an electron-releasing amino group in the 3'-position, produced the highest affinity. Compound I was also the most selective epibatidine analog with a Ki of 0.001 nM at αβ nAChRs, which is 26 times greater than that of epibatidine, and a αβ/α7 Ki ratio of 14 000, twice that of epibatidine. In vivo testing revealed that this compound potently inhibited nicotine-induced antinociception with AD50 values below 1 μg/kg. Surprisingly, this same compound was also an agonist at higher doses (ED50 .apprx.20 μg/kg). Thus, the addition of the 3'-amino group to epibatidine

confers potent antagonist activity to the compound with little effect on agonist activity. 2,3-Disubstituted epibatidine analogs possessing a 2'-amino group combined with a 3'-bromo or 3'-iodo group showed in vitro and in vivo nAChR properties similar to nicotine.

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(18) OF 95 ...N ===> AW

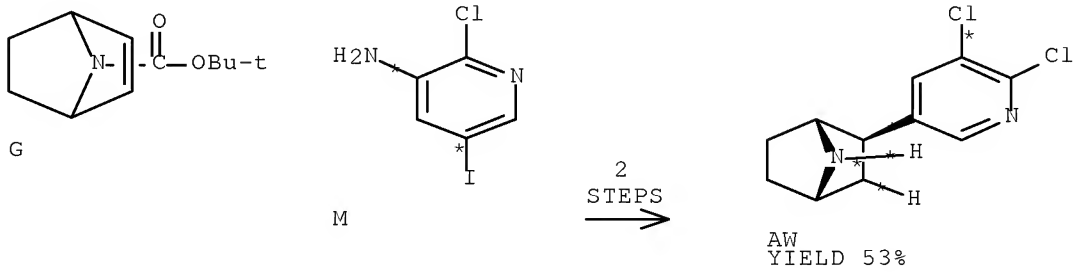


N

AW
YIELD 53%

RX(18) RCT N 426461-98-5
RGT X 7647-01-0 HCl, D 7632-00-0 NaNO2, Y 7758-89-6 CuCl
PRO AW 426460-53-9
SOL 7732-18-5 Water

RX(32) OF 95 COMPOSED OF RX(3), RX(18)
RX(32) G + M ===> AW



G

M

AW
YIELD 53%

RX(3) RCT G 192118-47-1, M 426463-09-4

STAGE(1)
RGT I 590-29-4 HCO2K
CAT 3375-31-3 Pd(OAc)2, 1112-67-0 Bu4NCl
SOL 68-12-2 DMF

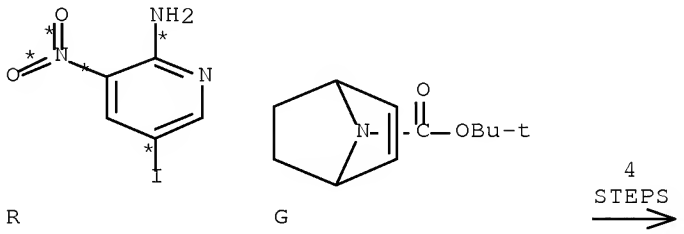
STAGE(2)
RGT E 1336-21-6 NH4OH
SOL 7732-18-5 Water

PRO N 426461-98-5

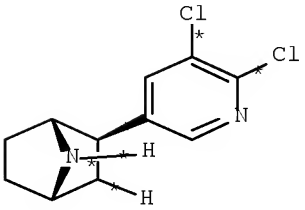
NTE stereoselective

RX(18) RCT N 426461-98-5
RGT X 7647-01-0 HCl, D 7632-00-0 NaNO2, Y 7758-89-6 CuCl
PRO AW 426460-53-9
SOL 7732-18-5 Water

RX(69) OF 95 COMPOSED OF RX(6), RX(8), RX(3), RX(18)
RX(69) R + G ===> AW



R G



AW
YIELD 53%

RX(6) RCT R 25391-57-5

STAGE(1)
RGT X 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(2)
RGT D 7632-00-0 NaNO2, Y 7758-89-6 CuCl

STAGE(3)
RGT E 1336-21-6 NH4OH
SOL 7732-18-5 Water

PRO W 426463-05-0

RX(8) RCT W 426463-05-0
RGT X 7647-01-0 HCl, AB 7439-89-6 Fe
PRO M 426463-09-4
SOL 64-17-5 EtOH, 7732-18-5 Water

RX(3) RCT G 192118-47-1, M 426463-09-4

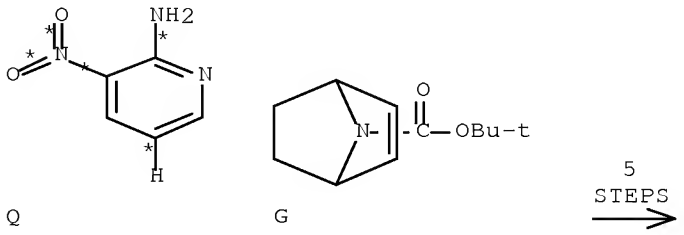
STAGE(1)
RGT I 590-29-4 HCO2K
CAT 3375-31-3 Pd(OAc)2, 1112-67-0 Bu4NCl
SOL 68-12-2 DMF

STAGE(2)
RGT E 1336-21-6 NH4OH
SOL 7732-18-5 Water

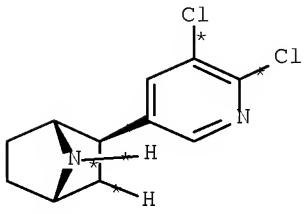
PRO N 426461-98-5
NTE stereoselective

RX(18) RCT N 426461-98-5
RGT X 7647-01-0 HCl, D 7632-00-0 NaNO2, Y 7758-89-6 CuCl
PRO AW 426460-53-9
SOL 7732-18-5 Water

RX(82) OF 95 COMPOSED OF RX(5), RX(6), RX(8), RX(3), RX(18)
RX(82) Q + G ===> AW



Q G



AW
YIELD 53%

RX(5) RCT Q 4214-75-9

STAGE(1)
RGT S 7553-56-2 I2
CAT 10450-60-9 H5IO6
SOL 64-19-7 AcOH, 7732-18-5 Water

STAGE(2)
RGT T 7772-98-7 Na2S2O3
SOL 7732-18-5 Water

PRO R 25391-57-5

RX(6) RCT R 25391-57-5

STAGE(1)
RGT X 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(2)
RGT D 7632-00-0 NaNO2, Y 7758-89-6 CuCl

STAGE(3)
RGT E 1336-21-6 NH4OH
SOL 7732-18-5 Water

PRO W 426463-05-0

RX(8) RCT W 426463-05-0
RGT X 7647-01-0 HCl, AB 7439-89-6 Fe
PRO M 426463-09-4
SOL 64-17-5 EtOH, 7732-18-5 Water

RX(3) RCT G 192118-47-1, M 426463-09-4

STAGE(1)
RGT I 590-29-4 HCO2K
CAT 3375-31-3 Pd(OAc)2, 1112-67-0 Bu4NCl
SOL 68-12-2 DMF

STAGE(2)
RGT E 1336-21-6 NH4OH
SOL 7732-18-5 Water

PRO N 426461-98-5
NTE stereoselective

RX(18) RCT N 426461-98-5
RGT X 7647-01-0 HCl, D 7632-00-0 NaNO2, Y 7758-89-6 CuCl
PRO AW 426460-53-9
SOL 7732-18-5 Water

L68 ANSWER 6 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:1369724 ZCAPLUS Full-text
DOCUMENT NUMBER: 150:19997
TITLE: Method for preparing 2,3-dichloropyridine
INVENTOR(S): Liu, Xiaomin
PATENT ASSIGNEE(S): Hebei Yanuo Chemical Industry Co., Ltd., Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 10pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 101302190	A	20081112	CN 2008-10055291	20080630
PRIORITY APPLN. INFO.:			CN 2008-10055291	20080630

AB The title method comprises the steps of: dissolving 3-aminopyridine into concentrated HCl acid to obtain a HCl acid solution of 3-aminopyridine hydrochloride, performing chlorination onto 3-aminopyridine with chlorinating agents with Fe2+ or Fe3+ as catalyst to obtain a system containing mainly 2-chloro-3-aminopyridine, performing diazotization/chlorination with sodium nitrite with Cu+ and/or Cu2+ as catalyst to obtain 2,3-dichloropyridine, adjusting the pH to above 7, distilling with water vapor to obtain crude 2,3-dichloropyridine, and recrystg. to obtain refined 2,3-dichloropyridine. The method has high product purity (above 99.2%), and high yield (above 71.4% calculated by 3-aminopyridine).

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))

ST dichloropyridine prepn aminopyridine diazotization chlorination catalyst iron copper salt

IT Diazotization catalysts
(copper salt; preparation of 2,3-dichloropyridine from 3-aminopyridine)

IT Chlorination catalysts
(iron/copper salt; preparation of 2,3-dichloropyridine from 3-aminopyridine)

IT 1317-38-0, Cupric oxide, uses 1317-39-1, Cuprous oxide, uses 7447-39-4, Cupric chloride, uses 7758-89-6, Cuprous chloride 17599-81-4, Cuprous sulfate
RL: CAT (Catalyst use); USES (Uses)
(diazotization/chlorination catalyst; preparation of 2,3-dichloropyridine from 3-aminopyridine)

IT 2402-77-9P, 2,3-Dichloropyridine
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of 2,3-dichloropyridine from 3-aminopyridine)

IT 462-08-8, 3-Aminopyridine
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 2,3-dichloropyridine from 3-aminopyridine)

IT 6298-19-7P, 2-Chloro-3-aminopyridine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2,3-dichloropyridine from 3-aminopyridine)

IT 7632-00-0, Sodium nitrite 7647-01-0, Hydrochloric acid, reactions 7722-84-1, Hydrogen peroxide (H2O2), reactions 7782-50-5, Chlorine, reactions
RL: RGT (Reagent); RACT (Reactant or reagent)
(preparation of 2,3-dichloropyridine from 3-aminopyridine)

IT 1317-38-0, Cupric oxide, uses 1317-39-1, Cuprous oxide, uses 7447-39-4, Cupric chloride, uses 7758-89-6, Cuprous chloride 17599-81-4, Cuprous sulfate
RL: CAT (Catalyst use); USES (Uses)
(diazotization/chlorination catalyst; preparation of 2,3-dichloropyridine from 3-aminopyridine)

RN 1317-38-0 ZCAPLUS

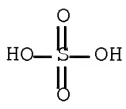
CN Copper oxide (CuO) (CA INDEX NAME)

RN 1317-39-1 ZCAPLUS
CN Copper oxide (Cu2O) (CA INDEX NAME)

RN 7447-39-4 ZCAPLUS
CN Copper chloride (CuCl2) (CA INDEX NAME)

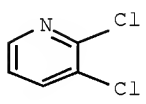
RN 7758-89-6 ZCAPLUS
CN Copper chloride (CuCl) (CA INDEX NAME)

RN 17599-81-4 ZCAPLUS
CN Sulfuric acid, copper(1+) salt (1:2) (CA INDEX NAME)

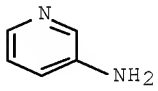


●2 Cu(I)

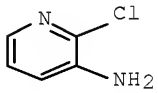
IT 2402-77-9P, 2,3-Dichloropyridine
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of 2,3-dichloropyridine from 3-aminopyridine)
RN 2402-77-9 ZCAPLUS
CN Pyridine, 2,3-dichloro- (CA INDEX NAME)



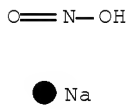
IT 462-08-8, 3-Aminopyridine
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 2,3-dichloropyridine from 3-aminopyridine)
RN 462-08-8 ZCAPLUS
CN 3-Pyridinamine (CA INDEX NAME)



IT 6298-19-7P, 2-Chloro-3-aminopyridine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(preparation of 2,3-dichloropyridine from 3-aminopyridine)
RN 6298-19-7 ZCAPLUS
CN 3-Pyridinamine, 2-chloro- (CA INDEX NAME)



IT 7632-00-0, Sodium nitrite
RL: RGT (Reagent); RACT (Reactant or reagent)
(preparation of 2,3-dichloropyridine from 3-aminopyridine)
RN 7632-00-0 ZCAPLUS
CN Nitrous acid, sodium salt (1:1) (CA INDEX NAME)

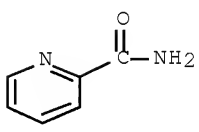


L68 ANSWER 7 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:1287458 ZCAPLUS Full-text
DOCUMENT NUMBER: 146:183995
TITLE: Cu(I)-mediated deoxygenation of N-oxides to amines
AUTHOR(S): Singh, Sunil Kumar; Reddy, M. Srinivasa; Mangle, Mangesh; Ganesh, K. Ravi
CORPORATE SOURCE: Discovery Chemistry, Discovery Research-Dr. Reddy's Laboratories Ltd., Hyderabad, 500 049, India
SOURCE: Tetrahedron (2006), Volume Date 2007, 63(1), 126-130
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal

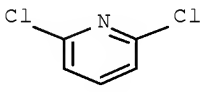
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:183995
AB A mild and highly efficient deoxygenation of variety of N-oxides using an inexpensive CuX (X = I, Cl) or a CuX-Zn or CuX-Al couple is described. Though CuX alone effectively deoxygenates the aliphatic and aromatic N-oxides in aprotic solvents at lower temperature (30-50°C), the CuX-Zn and CuX-Al systems require refluxing the substrates (viz., nitrone, azoxybenzene, and heteroarene N-oxides) in ethanol at 50-60°C.
CC 21-2 (General Organic Chemistry)
IT 7429-90-5, Aluminum, uses 7440-66-6, Zinc, uses 7681-65-4, Copper iodide (CuI) 7758-89-6, Copper chloride (CuCl)
RL: CAT (Catalyst use); USES (Uses)
(preparation of amines by Cu(I)-mediated deoxygenation of N-oxides)
IT 91-22-5P, Quinoline, preparation 91-63-4P, 2-Methylquinoline 109-02-4P, 4-Methylmorpholine 109-06-8P, 2-Methylpyridine 109-09-1P, 2-Chloropyridine 110-86-1P, Pyridine, preparation 121-44-8P, Triethylamine, preparation 612-62-4P, 2-Chloroquinoline 702-11-4P 824-21-5P 933-94-8P 1452-77-3P, 2-Pyridinecarboxamide 2402-78-0P, 2,6-Dichloropyridine 2459-07-6P, Methyl 2-pyridinecarboxylate 2632-65-7P 10220-22-1P 16155-03-6P 39769-11-4P 123330-59-6P 329943-64-8P 385380-74-5P 922142-73-2P 922142-74-3P 922142-75-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of amines by Cu(I)-mediated deoxygenation of N-oxides)
IT 7681-65-4, Copper iodide (CuI) 7758-89-6, Copper chloride (CuCl)
RL: CAT (Catalyst use); USES (Uses)
(preparation of amines by Cu(I)-mediated deoxygenation of N-oxides)
RN 7681-65-4 ZCAPLUS
CN Copper iodide (CuI) (CA INDEX NAME)

RN 7758-89-6 ZCAPLUS
CN Copper chloride (CuCl) (CA INDEX NAME)

IT 1452-77-3P, 2-Pyridinecarboxamide 2402-78-0P, 2,6-Dichloropyridine
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of amines by Cu(I)-mediated deoxygenation of N-oxides)
RN 1452-77-3 ZCAPLUS
CN 2-Pyridinecarboxamide (CA INDEX NAME)



RN 2402-78-0 ZCAPLUS
CN Pyridine, 2,6-dichloro- (CA INDEX NAME)



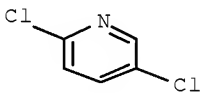
REFERENCE COUNT: 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L68 ANSWER 8 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:270415 ZCAPLUS Full-text
DOCUMENT NUMBER: 134:266210
TITLE: Preparation of 2,5-dichloropyridine from 2-amino-5-chloropyridine
INVENTOR(S): Yokota, Keiichi; Takeuchi, Seiji
PATENT ASSIGNEE(S): Sumikin Chemical K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

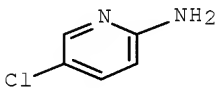
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001106672	A	20010417	JP 1999-284819	19991005

PRIORITY APPLN. INFO.: JP 1999-284819 19991005
OTHER SOURCE(S): CASREACT 134:266210
AB 2,5-Dichloropyridine (I) is prepared by treatment of 2-amino-5-chloropyridine (II) with NaNO2 in HCl, and the byproduct, 5-chloro-2-hydroxypyridine (III) is further treated with POCl3 in the presence of DMF. Thus, II was treated with aqueous NaNO2 at 40-50° in HCl-MePh, neutralized, and filtered to give crystals containing III. The organic phase of the filtrate was mixed with the crystals, evaporated to dryness, mixed with DMF, and treated with POCl3 at 100° to give I with 84.5% yield from II.
IC ICM C07D213-61
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
IT 16110-09-1P, 2,5-Dichloropyridine
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(Preparation of 2,5-dichloropyridine from 2-amino-5-chloropyridine)
IT 1072-98-6, 2-Amino-5-chloropyridine 7632-00-0, Sodium nitrite 7647-01-0, Hydrochloric acid, reactions 10025-87-3, Phosphorus oxychloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(Preparation of 2,5-dichloropyridine from 2-amino-5-chloropyridine)
IT 16110-09-1P, 2,5-Dichloropyridine
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(Preparation of 2,5-dichloropyridine from 2-amino-5-chloropyridine)
RN 16110-09-1 ZCAPLUS

CN Pyridine, 2,5-dichloro- (CA INDEX NAME)



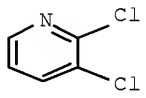
IT 1072-98-6, 2-Amino-5-chloropyridine
RL: RCT (Reactant); RACT (Reactant or reagent)
(Preparation of 2,5-dichloropyridine from 2-amino-5-chloropyridine)
RN 1072-98-6 ZCAPLUS
CN 2-Pyridinamine, 5-chloro- (CA INDEX NAME)



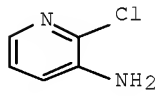
L68 ANSWER 9 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:314380 ZCAPLUS Full-text
DOCUMENT NUMBER: 125:33445
ORIGINAL REFERENCE NO.: 125:6529a,6532a
TITLE: Substituent effect on the chlorination of 2-alkoxypyridines to give 2-chloropyridines under Vilsmeier-Haack conditions
AUTHOR(S): Lai, Long-Li; Lin, Pen-Yuan; Wang, Jy-Shih; Hwu, Jih Ru; Shiao, Min-Jen; Tsay, Shwu-Chen
CORPORATE SOURCE: Inst. Chem., Acad. Sinica, Taipei, 11529, Taiwan
SOURCE: Journal of Chemical Research, Synopses (1996), (4), 194-195
CODEN: JRPSDC; ISSN: 0308-2342
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:33445
AB Various substituted 2-alkoxypyridines were converted into the corresponding 2-chloropyridines in 28-91% yield by use of POCl3 and DMF. Me, halogen, ester and nitro groups displayed an activating effect and an amino group exhibited a deactivating effect.
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
IT 109-09-1P, 2-Chloropyridine 2402-77-9P, 2,3-Dichloropyridine 2402-78-0P, 2,6-Dichloropyridine 4548-45-2P, 2-Chloro-5-nitropyridine 5140-72-7P, 2-Bromo-6-chloropyridine 5470-18-8P, 2-Chloro-3-nitropyridine 6298-19-7P, 3-Amino-2-chloropyridine 18368-63-3P, 2-Chloro-6-methylpyridine 52200-48-3P, 3-Bromo-2-chloropyridine 73781-91-6P, Methyl 6-chloro-3-pyridinecarboxylate
RL: SPN (Synthetic preparation); PREP (Preparation)
(substituent effect on the chlorination of 2-alkoxypyridines to give 2-chloropyridines under Vilsmeier-Haack conditions)
IT 2402-77-9P, 2,3-Dichloropyridine 6298-19-7P, 3-Amino-2-chloropyridine

RL: SPN (Synthetic preparation); PREP (Preparation)
(substituent effect on the chlorination of 2-alkoxypyridines to give 2-chloropyridines under Vilsmeier-Haack conditions)

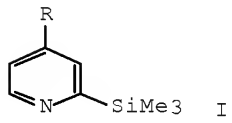
RN 2402-77-9 ZCAPLUS
CN Pyridine, 2,3-dichloro- (CA INDEX NAME)



RN 6298-19-7 ZCAPLUS
CN 3-Pyridinamine, 2-chloro- (CA INDEX NAME)



L68 ANSWER 10 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1992:407994 ZCAPLUS Full-text
DOCUMENT NUMBER: 117:7994
ORIGINAL REFERENCE NO.: 117:1619a,1622a
TITLE: Electrophilic aromatic substitution. 39. The mechanism of the carbodesilylation of 4- or 5-substituted 2-(trimethylsilyl)pyridines
AUTHOR(S): Effenberger, Franz; Krebs, Andreas; Willrett, Peter
CORPORATE SOURCE: Inst. Org. Chem., Univ. Stuttgart, Stuttgart, W-7000/80, Germany
SOURCE: Chemische Berichte (1992), 125(5), 1131-40
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



I

AB An ylide mechanism is proposed for the carbodesilylation of 2-(trimethylsilyl)pyridines with benzaldehyde. In contrast, 3- and 4-(trimethylsilyl)pyridines (e.g., I; R = H, Me, MeO, Cl, CN, PhSO2, Me3Si) react only in the presence of a base catalyst via pyridyl anions with electrophiles. The rates of the uncatalyzed carbodesilylation reactions of I

with benzaldehyde correlate very well with the resonance parameters of the substituents σR0, whereas the rates of 5-substituted 2-(trimethylsilyl)pyridines correlate with the inductive substituent parameters σI in the Taft equation. This is the first direct determination of the resonance parameters σR0.

CC 29-6 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 22

IT 695-34-1 1072-98-6 1603-41-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(bromination of)

IT 504-29-0, 2-Aminopyridine
RL: RCT (Reactant); RACT (Reactant or reagent)
(iodination of)

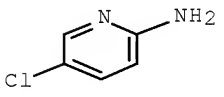
IT 5350-93-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amination of)

IT 1453-82-3P, 4-Pyridinecarboxamide 4214-76-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)

IT 3510-66-5P 4926-28-7P 22918-01-0P 26452-80-2P 33252-28-7P 33252-30-1P 40473-01-6P 67743-63-9P 89488-29-9P 139585-48-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and silylation of)

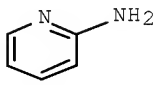
IT 1072-98-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(bromination of)

RN 1072-98-6 ZCAPLUS
CN 2-Pyridinamine, 5-chloro- (CA INDEX NAME)



IT 504-29-0, 2-Aminopyridine
RL: RCT (Reactant); RACT (Reactant or reagent)
(iodination of)

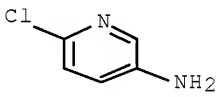
RN 504-29-0 ZCAPLUS
CN 2-Pyridinamine (CA INDEX NAME)



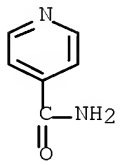
IT 5350-93-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amination of)

RN 5350-93-6 ZCAPLUS

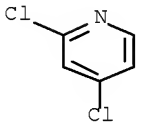
CN 3-Pyridinamine, 6-chloro- (CA INDEX NAME)



IT 1453-82-3P, 4-Pyridinecarboxamide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)
RN 1453-82-3 ZCAPLUS
CN 4-Pyridinecarboxamide (CA INDEX NAME)



IT 26452-80-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and silylation of)
RN 26452-80-2 ZCAPLUS
CN Pyridine, 2,4-dichloro- (CA INDEX NAME)



L68 ANSWER 11 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1989:192171 ZCAPLUS Full-text
DOCUMENT NUMBER: 110:192171
ORIGINAL REFERENCE NO.: 110:31881a,31884a
TITLE: Site selectivity in the reaction of 3-substituted pyridine 1-oxides with phosphoryl chloride
AUTHOR(S): Yamanaka, Hiroshi; Araki, Tomio; Sakamoto, Takao
CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, 980, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1988), 36(6), 2244-7
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:192171

AB Site selectivity in the reaction of 3-substituted pyridine 1-oxides with phosphoryl chloride was investigated. When a strongly electron-withdrawing group e.g., (CN, CONRR', CO2R, NO2) was substituted at the 3-position, the reaction of 3-substituted pyridine 1-oxides with phosphoryl chloride yielded 3-substituted 2-chloropyridines as the main products.

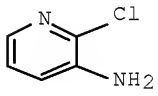
CC 22-13 (Physical Organic Chemistry)
Section cross-reference(s): 29

IT 6298-19-7, 3-Amino-2-chloropyridine
RL: PROC (Process)
(conversion of, to chloro(dimethylamino)pyridine)

IT 109-09-1P 626-61-9P 1452-94-4P 1681-36-3P 2402-77-9P
4548-45-2P 5470-18-8P 6602-54-6P 13091-23-1P 16110-09-1P
18368-64-4P 18368-76-8P 19069-63-7P 31557-57-0P 33252-28-7P
36953-42-1P 37831-62-2P 38029-99-1P 41288-91-9P 49608-01-7P
52200-48-3P 53939-30-3P 54864-96-9P 55675-97-3P 55934-00-4P
66600-05-3P 89284-61-7P 120234-29-9P 120234-30-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

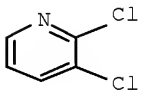
IT 6298-19-7, 3-Amino-2-chloropyridine
RL: PROC (Process)
(conversion of, to chloro(dimethylamino)pyridine)

RN 6298-19-7 ZCAPLUS
CN 3-Pyridinamine, 2-chloro- (CA INDEX NAME)



IT 2402-77-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 2402-77-9 ZCAPLUS
CN Pyridine, 2,3-dichloro- (CA INDEX NAME)



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=>  d his full

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     FILE 'ZCAPLUS' ENTERED AT 11:56:38 ON 06 MAR 2009

     FILE 'ZCAPLUS' ENTERED AT 11:56:54 ON 06 MAR 2009
L1             1 SEA SPE=ON  ABB=ON  PLU=ON  US2006-583635/APPS
                 D SCA
                 SEL RN

     FILE 'REGISTRY' ENTERED AT 11:57:51 ON 06 MAR 2009
L2             9 SEA SPE=ON  ABB=ON  PLU=ON  (1317-38-0/BI OR 2402-77-9/BI OR
                 462-08-8/BI OR 6298-19-7/BI OR 73074-20-1/BI OR 7447-39-4/BI
                 OR 7632-00-0/BI OR 94770-75-9/BI OR 98-92-0/BI)
L3             1 SEA SPE=ON  ABB=ON  PLU=ON  2402-77-9
                 D SCA
                 D SCA L2
L4             6 SEA SPE=ON  ABB=ON  PLU=ON  L2 AND NC5/ES
                 D SCA
L5             5 SEA SPE=ON  ABB=ON  PLU=ON  L4 NOT  L3

     FILE 'ZCAPLUS' ENTERED AT 12:01:09 ON 06 MAR 2009
L6            23 SEA SPE=ON  ABB=ON  PLU=ON  L3 (L) PREP/RL
L7             5 SEA SPE=ON  ABB=ON  PLU=ON  L5 AND L6
                 D SCA

     FILE 'REGISTRY' ENTERED AT 12:02:06 ON 06 MAR 2009
L8             1 SEA SPE=ON  ABB=ON  PLU=ON  2402-77-9/CRN
                 D SCA
                 SEL RN L5
L9           572 SEA SPE=ON  ABB=ON  PLU=ON  (462-08-8/CRN OR 6298-19-7/CRN OR
                 73074-20-1/CRN OR 94770-75-9/CRN OR 98-92-0/CRN)
L10            2 SEA SPE=ON  ABB=ON  PLU=ON  L8 OR L3
L11          575 SEA SPE=ON  ABB=ON  PLU=ON  L9 OR L5

     FILE 'ZCAPLUS' ENTERED AT 12:03:24 ON 06 MAR 2009
L12           23 SEA SPE=ON  ABB=ON  PLU=ON  L10 (L) PREP/RL
L13            5 SEA SPE=ON  ABB=ON  PLU=ON  L11 AND L12
                 D SCA

     FILE 'REGISTRY' ENTERED AT 12:04:32 ON 06 MAR 2009
L14       544228 SEA SPE=ON  ABB=ON  PLU=ON  CU/ELS

     FILE 'ZCAPLUS' ENTERED AT 12:04:50 ON 06 MAR 2009
L15              TRA PLU=ON  L13 1- RN :      99 TERMS

     FILE 'REGISTRY' ENTERED AT 12:04:51 ON 06 MAR 2009
L16           99 SEA SPE=ON  ABB=ON  PLU=ON  L15
L17            5 SEA SPE=ON  ABB=ON  PLU=ON  L14 AND L16
L*** DEL  14673 S ?NITRIT?/BI
L18       14680 SEA SPE=ON  ABB=ON  PLU=ON  ?NITRIT?/CNS
L19            1 SEA SPE=ON  ABB=ON  PLU=ON  L16 AND L18
                 D SCA
L20           32 SEA SPE=ON  ABB=ON  PLU=ON  L16 AND NC5/ESS AND N>1
                 D SCA

     FILE 'ZCAPLUS' ENTERED AT 12:06:54 ON 06 MAR 2009
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L21           2 SEA SPE=ON  ABB=ON  PLU=ON  L13 AND (L17 OR L19)
L22           3 SEA SPE=ON  ABB=ON  PLU=ON  L13 AND (CU/BI OR COPPER?/BI OR
                CUPR?/BI)

     FILE 'REGISTRY' ENTERED AT 12:09:01 ON 06 MAR 2009
                D SCA L3
L23          16 SEA SPE=ON  ABB=ON  PLU=ON  C5H3CL2N/MF
                D SCA

     FILE 'ZCAPLUS' ENTERED AT 12:10:01 ON 06 MAR 2009
L24         163 SEA SPE=ON  ABB=ON  PLU=ON  L23 (L) PREP/RL
L25           5 SEA SPE=ON  ABB=ON  PLU=ON  L5 AND L24

     FILE 'REGISTRY' ENTERED AT 12:11:15 ON 06 MAR 2009
                SEL RN L23
L26         109 SEA SPE=ON  ABB=ON  PLU=ON  (1001003-85-5/CRN OR 1001003-86-6/C
                RN OR 1001003-87-7/CRN OR 1001003-88-8/CRN OR 1001003-91-3/CRN
                OR 1001003-97-9/CRN OR 16110-09-1/CRN OR 2402-77-9/CRN OR
                2402-78-0/CRN OR 2457-47-8/CRN OR 25586-45-2/CRN OR 26452-80-2/
                CRN OR 55934-00-4/CRN OR 70735-32-9/CRN OR 851516-88-6/CRN OR
                98136-41-5/CRN)
L27         125 SEA SPE=ON  ABB=ON  PLU=ON  L23 OR L26
                D SCA L5
                SEL MF L5
L28         571 SEA SPE=ON  ABB=ON  PLU=ON  (C5H5CLN2.CLH/MF OR C5H5CLN2/MF OR
                C5H6N2.CLH/MF OR C5H6N2/MF OR C6H6N2O/MF)
L29         151 SEA SPE=ON  ABB=ON  PLU=ON  L28 AND NC5/ES
L30         151 SEA SPE=ON  ABB=ON  PLU=ON  L5 OR L29

     FILE 'ZCAPLUS' ENTERED AT 12:13:52 ON 06 MAR 2009
L31         209 SEA SPE=ON  ABB=ON  PLU=ON  L27 (L) PREP/RL
L32          23 SEA SPE=ON  ABB=ON  PLU=ON  L30 AND L31

     FILE 'REGISTRY' ENTERED AT 12:15:52 ON 06 MAR 2009

     FILE 'ZCAPLUS' ENTERED AT 12:16:02 ON 06 MAR 2009
L33             TRA PLU=ON  L32 1- RN :    7677 TERMS

     FILE 'REGISTRY' ENTERED AT 12:16:07 ON 06 MAR 2009
L34        7677 SEA SPE=ON  ABB=ON  PLU=ON  L33
L35           6 SEA SPE=ON  ABB=ON  PLU=ON  L34 AND L14

     FILE 'ZCAPLUS' ENTERED AT 12:16:58 ON 06 MAR 2009
L36           3 SEA SPE=ON  ABB=ON  PLU=ON  L32 AND L35
L37           7 SEA SPE=ON  ABB=ON  PLU=ON  L32 AND (CU/BI OR COPPER?/BI OR
                CUPR?/BI)
                D SCA
L38        9735 SEA SPE=ON  ABB=ON  PLU=ON  L30 (L) RACT/RL
L39           3 SEA SPE=ON  ABB=ON  PLU=ON  L38 AND L37
L40           4 SEA SPE=ON  ABB=ON  PLU=ON  L37 NOT L39
                D SCA
                D SCA L39
L41           3 SEA SPE=ON  ABB=ON  PLU=ON  L13 AND L39

     FILE 'REGISTRY' ENTERED AT 12:23:58 ON 06 MAR 2009
L42         721 SEA SPE=ON  ABB=ON  PLU=ON  L11 OR L29
L43         721 SEA SPE=ON  ABB=ON  PLU=ON  L42 AND NC5/ES

     FILE 'ZCAPLUS' ENTERED AT 12:24:31 ON 06 MAR 2009
L44          24 SEA SPE=ON  ABB=ON  PLU=ON  L43 AND L31
```

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L45           1 SEA SPE=ON  ABB=ON  PLU=ON  L44 NOT L32
                D SCA
L46     1219793 SEA SPE=ON  ABB=ON  PLU=ON  TRANSITION?/BI
L47           0 SEA SPE=ON  ABB=ON  PLU=ON  L44 AND L46
                E COPPER+ALL/CT
L48           0 SEA SPE=ON  ABB=ON  PLU=ON  L44 AND GROUP IB/BI
L49           9 SEA SPE=ON  ABB=ON  PLU=ON  L44 AND ?DIAZ?/BI
L*** DEL      0 S L43 (L) RACT
L50        9763 SEA SPE=ON  ABB=ON  PLU=ON  L43 (L) RACT/RL
L51           5 SEA SPE=ON  ABB=ON  PLU=ON  L50 AND L31
                D SCA

     FILE 'CASREACT' ENTERED AT 12:34:23 ON 06 MAR 2009
L52             STRUCTURE UPLOADED
L53           7 SEA SSS SAM L52 (    92 REACTIONS)
                D SCA
                D STAT QUE

     FILE 'REGISTRY' ENTERED AT 12:35:35 ON 06 MAR 2009
L54       30743 SEA SPE=ON  ABB=ON  PLU=ON  CU/ELS AND CASREACT/LC

     FILE 'CASREACT' ENTERED AT 12:35:51 ON 06 MAR 2009
L55       51052 SEA SPE=ON  ABB=ON  PLU=ON  L54
L56           0 SEA SUB=L55 SSS SAM L52 (     0 REACTIONS)
L57          12 SEA SUB=L55 SSS FUL L52 (    77 REACTIONS)
                D SCA

     FILE 'ZCAPLUS' ENTERED AT 12:38:54 ON 06 MAR 2009

     FILE 'CASREACT' ENTERED AT 12:39:12 ON 06 MAR 2009
                D OCC L57 1-

     FILE 'ZCAPLUS' ENTERED AT 12:39:16 ON 06 MAR 2009

     FILE 'CASREACT' ENTERED AT 12:39:43 ON 06 MAR 2009
                D HIT L57 4
L58             STRUCTURE UPLOADED

     FILE 'CASREACT' ENTERED AT 12:41:20 ON 06 MAR 2009
L59           0 SEA SUB=L57 SSS SAM L58 (     0 REACTIONS)
L60           5 SEA SUB=L57 SSS FUL L58 (    12 REACTIONS)
                D SCA
L61           7 SEA SPE=ON  ABB=ON  PLU=ON  L57 NOT L60
                D SCA

     FILE 'ZCAPLUS' ENTERED AT 12:43:15 ON 06 MAR 2009
L62         866 SEA SPE=ON  ABB=ON  PLU=ON  SHAPIRO R?/AU
L63           1 SEA SPE=ON  ABB=ON  PLU=ON  L62 AND L31
                D SCA
L64           4 SEA SPE=ON  ABB=ON  PLU=ON  (L27 OR L43) AND L62
                D SCA
                D SCA

     FILE 'REGISTRY' ENTERED AT 12:46:08 ON 06 MAR 2009

     FILE 'ZCAPLUS' ENTERED AT 12:46:11 ON 06 MAR 2009
                D STAT QUE L64
                D IBIB ABS HITSTR L64 1-4

     FILE 'REGISTRY' ENTERED AT 12:47:00 ON 06 MAR 2009
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     FILE 'ZCAPLUS' ENTERED AT 12:47:04 ON 06 MAR 2009
                D STAT QUE L13
                D STAT QUE L21
                D STAT QUE L22
                D STAT QUE L36
                D STAT QUE L39
                D STAT QUE L51
L65           8 SEA SPE=ON  ABB=ON  PLU=ON  L13 OR L21 OR L22 OR L36 OR L51 OR
                L39

     FILE 'CASREACT' ENTERED AT 12:47:51 ON 06 MAR 2009
                D STAT QUE L60

     FILE 'CASREACT, ZCAPLUS' ENTERED AT 12:48:04 ON 06 MAR 2009
L66          11 DUP REM L60 L65 (2 DUPLICATES REMOVED)
                    ANSWERS '1-5' FROM FILE CASREACT
                    ANSWERS '6-11' FROM FILE ZCAPLUS

     FILE 'CASREACT' ENTERED AT 12:48:40 ON 06 MAR 2009
L67           5 SEA SPE=ON  ABB=ON  PLU=ON  L55 (L) L60
                D STAT QUE L67

     FILE 'CASREACT, ZCAPLUS' ENTERED AT 12:49:21 ON 06 MAR 2009
L68          11 DUP REM L67 L65 (2 DUPLICATES REMOVED)
                    ANSWERS '1-5' FROM FILE CASREACT
                    ANSWERS '6-11' FROM FILE ZCAPLUS
                D IBIB ABS HIT L68 1-5
                D IBIB ABS HITIND HITSTR L68 6-11


     FILE HOME

     FILE ZCAPLUS

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     FILE COVERS 1907 - 6 Mar 2009  VOL 150 ISS 11
     FILE LAST UPDATED: 5 Mar 2009  (20090305/ED)

     ZCAplus now includes complete International Patent Classification (IPC)
     reclassification data for the third quarter of 2008.

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     http://www.cas.org/legal/infopolicy.html

     This file contains CAS Registry Numbers for easy and accurate
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     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
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DICTIONARY FILE UPDATES: 4 MAR 2009 HIGHEST RN 1115640-24-8

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FILE CASREACT

FILE CONTENT:1840 - 2 Mar 2009 VOL 150 ISS 10

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This file contains CAS Registry Numbers for easy and accurate substance identification.
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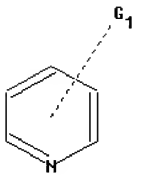
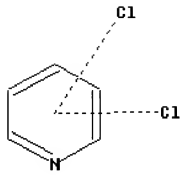
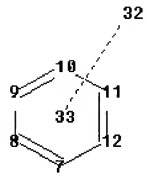
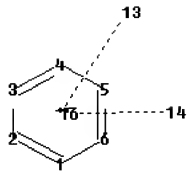
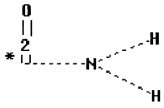
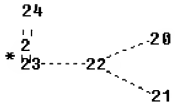


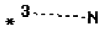


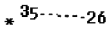










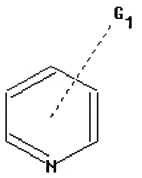


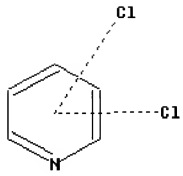
chain nodes :
13 14 17 18 19 20 21 22 23 24 25 26 32
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
17-18 17-19 20-22 21-22 22-23 23-24 25-26
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
17-18 17-19 20-22 21-22 22-23 23-24 25-26
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

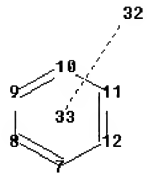
G1:[*1],[*2],[*3]

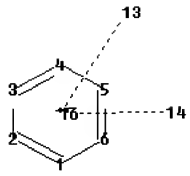
Connectivity :
25:2 E exact RC ring/chain 26:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 32:CLASS 33:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 7
node mappings:
1:7

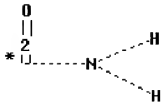
Uploading L58.str

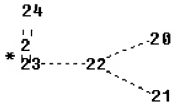


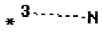


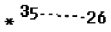












chain nodes :
13 14 17 18 19 20 21 22 23 24 25 26 32
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
17-18 17-19 20-22 21-22 22-23 23-24 25-26
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
17-18 17-19 20-22 21-22 22-23 23-24 25-26
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

G1:[*1],[*2],[*3]

Connectivity :
25:2 E exact RC ring/chain 26:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 32:CLASS 33:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 7
reaction site bonds:
13-15:CC
node mappings:
1:7

=>